Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquamanganese(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate

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Received 30 November 2004
Accepted 3 December 2004
Online 11 December 2004

Key indicators

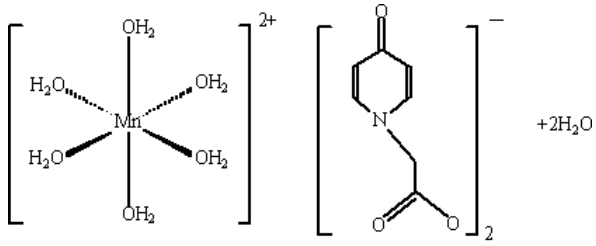
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.085
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $[Mn(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$, was synthesized by the reaction of $MnCl_2\cdot 4H_2O$ and (4-oxo-4*H*-pyrindin-1-yl)acetic acid in aqueous solution. The manganese(II) ion, which lies on a center of symmetry, is octahedrally coordinated by six water molecules [Mn—O = 2.166 (1)–2.177 (1) Å]. A three-dimensional supramolecular framework is formed *via* O—H···O hydrogen bonds between the anions and cations.

Comment

A recent study documented the structure of the complexes $[M(H_2O)_6](4\text{-OPA})_2\cdot 2H_2O$ [M = Zn, Ni; 4-OPA is (4-oxo-4*H*-pyridin-1-yl)acetate] (Gao *et al.*, 2004; Zhang *et al.*, 2004). The manganese(II) analogue was synthesized under similar reaction conditions in this study. The title complex, (I) (Fig. 1), in which Mn lies on a center of symmetry, is isomorphous with the Zn^{II} and Ni^{II} complexes, whose structures have been presented in detail.



(I)

Experimental

The title complex was prepared by the addition of $MnCl_2\cdot 4H_2O$ (3.96 g, 20 mmol) to an aqueous solution of (4-oxo-4*H*-pyridin-1-yl)acetic acid (5.84 g, 40 mmol), and the pH was adjusted to 7 with 0.2 *M* NaOH solution. Colorless single crystals were obtained from the filtered solution over several days. Analysis calculated for $[Mn(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$: C 33.41, H 5.61, N 5.57%; found: C 33.29, H 5.50, N 5.68%.

Crystal data

$[Mn(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$
M_r = 503.32
Monoclinic, $P2_1/c$
a = 12.561 (3) Å
b = 12.949 (3) Å
c = 6.855 (1) Å
β = 98.68 (3)°
V = 1102.2 (4) Å^3
Z = 2
D_x = 1.517 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 242 reflections
θ = 3.0–27.5°
μ = 0.67 mm^{-1}
T = 296 (2) K
Prism, colorless
0.39 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.780, T_{max} = 0.883
10 259 measured reflections
2509 independent reflections
2273 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -16 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.04
2509 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.3365P]$ where $P(F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1*w*	2.177 (1)	O2—C7	1.241 (2)
Mn1—O2*w*	2.166 (1)	O3—C3	1.280 (2)
Mn1—O3*w*	2.167 (1)	C1—C2	1.360 (2)
O1—C7	1.265 (2)	C4—C5	1.356 (2)
O2*w*—Mn1—O1*w*	91.64 (6)	O3*w*—Mn1—O1*w*	89.51 (5)
O2*w*—Mn1—O1*w*^{i}	88.36 (6)	O3*w*—Mn1—O1*w*^{i}	90.49 (5)
O2*w*—Mn1—O3*w*	89.27 (5)	N1—C6—C7	113.9 (1)
O2*w*—Mn1—O3*w*^{i}	90.73 (5)		

Symmetry code: (i) $-x, -y+1, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4*w*^{ii}	0.85 (2)	1.878 (11)	2.727 (2)	175 (2)
O1*w*—H1*w*2···O1^{ii}	0.85 (2)	1.99 (2)	2.831 (2)	167 (2)
O2*w*—H2*w*1···O2^{i}	0.84 (2)	1.85 (2)	2.698 (2)	176 (2)
O2*w*—H2*w*2···O3^{iii}	0.85 (2)	1.89 (2)	2.728 (2)	174 (3)
O3*w*—H3*w*1···O1	0.86 (2)	1.84 (2)	2.687 (2)	171 (2)
O3*w*—H3*w*2···O1^{iv}	0.86 (2)	2.03 (2)	2.835 (2)	155 (2)
O4*w*—H4*w*1···O3^{iii}	0.86 (2)	2.22 (3)	3.007 (2)	154 (3)
O4*w*—H4*w*2···O3^{v}	0.86 (2)	1.99 (3)	2.804 (2)	158 (3)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x+1, y, z$.

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C), and were included in the refinement in the riding-model approximation. H atoms of water molecules were located in Fourier difference maps and refined with the restraints O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, and with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

We thank the National Natural Science Foundation of China (No. 20101003), Heilongjiang Province Natural Science Foundation (No. B0007), Educational Committee Foundation of Heilongjiang Province and Heilongjiang University.

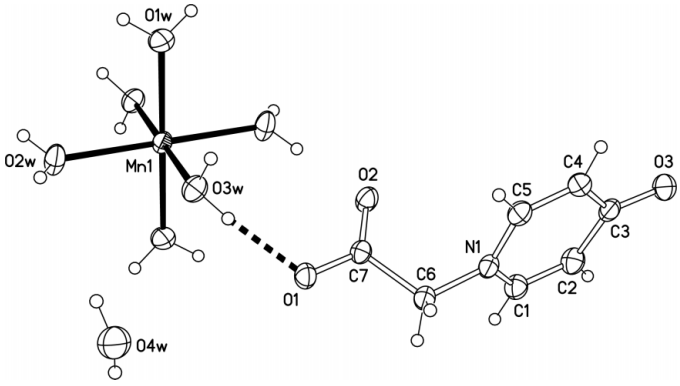


Figure 1
A view of complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The hydrogen bond is shown as a dashed line.

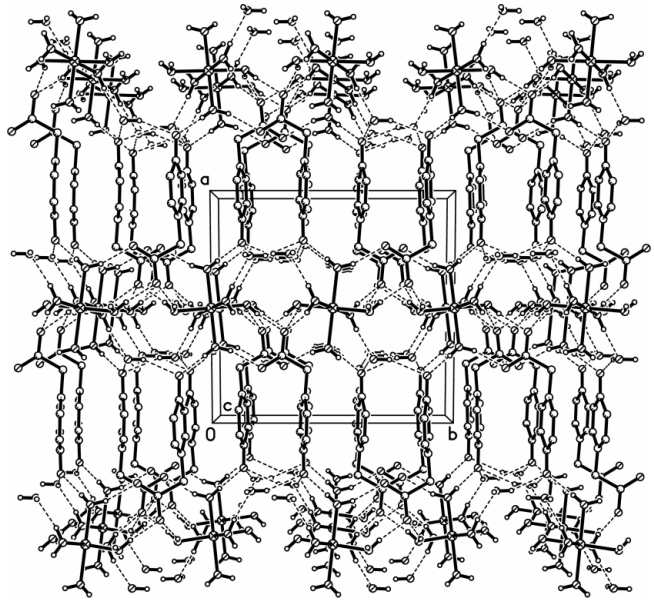


Figure 2
Packing diagram of the complex (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. C-bound H atoms have been omitted for clarity.

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